2-Methylphenoxathiin

Inchi: InChI=1S/C13H10OS/c1-9-6-7-11-13(8-9)15-12-5-3-2-4-10(12)14-11/h2-8H,1H3
InchiKey: BHEPNKKGEJFULV-UHFFFAOYSA-N
Formula: C13H10OS
SMILES: Cc1ccc2c(c1)Sc1ccccc1O2
Mol. weight [g/mol]: 214.28
CAS: 6103-33-9

Physical Properties

Property code	Value	Unit	Source
gf	288.81	kJ/mol	Joback Method
hf	139.56	kJ/mol	Joback Method
hfus	27.14	kJ/mol	Joback Method
hvap	61.44	kJ/mol	Joback Method
ie	7.78	eV	NIST Webbook
log10ws	-4.24		Crippen Method
logp	4.252		Crippen Method
mcvol	157.870	ml/mol	McGowan Method
pc	3356.75	kPa	Joback Method
tb	647.06	K	Joback Method
tc	912.18	K	Joback Method
tf	462.39	K	Joback Method
vc	0.581	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	376.86	J/mol×K	647.06	Joback Method
cpg	390.43	J/mol×K	691.25	Joback Method
cpg	402.85	J/mol×K	735.43	Joback Method
cpg	414.26	J/mol×K	779.62	Joback Method
cpg	424.79	J/mol×K	823.81	Joback Method
cpg	434.60	J/mol×K	868.00	Joback Method
cpg	443.82	J/mol×K	912.18	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6103339&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume